

Generating connected and biconnected graphs

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Abstract

We focus on the algorithm underlying the main result of [6]. This is an algebraic formula to generate all connected graphs in a recursive and efficient manner. The key feature is that each graph carries a scalar factor given by the inverse of the order of its group of automorphisms. In the present paper, we revise that algorithm on the level of graphs. Moreover, we extend the result subsequently to further classes of connected graphs, namely, (edge) biconnected, simple and loopless graphs. Our method consists of basic graph transformations only.

The present paper is part of a program laid out in [5, 6] with the focus on the combinatorics of different kinds of connected graphs and problems of graph generation. In particular, the main result of [5] is a recursion formula to generate all trees. This result is generalized to all connected graphs in [6]. The underlying structure is a Hopf algebraic representation of graphs. In both cases, in a recursion step, the formulas yield linear combinations of graphs with rational coefficients. The essential property is that the coefficients of graphs are given by the inverses of the orders of their groups of automorphisms. Other problems in this context are considered in [3, 7], for instance.

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In this paper, we express the algebraic recursion formula to generate all connected graphs given in [6], in terms of graphs. Moreover, we extend this result successively to (edge) biconnected, simple and loopless (connected) graphs. Crucially, as in [5, 6], the exact coefficients of graphs are obtained.

Our method is based on three linear graph transformations to produce a graph with, say, m edges from a graph with $m - 1$ edges. Namely, (a) assigning a loop to a vertex; (b) connecting a pair of vertices with an edge; (c) splitting a vertex in two, distributing the ends of edges assigned to the split vertex, between the two new ones in a given way, and connecting the two new vertices with an edge. In particular, the last operation is (equivalently) defined for simple graphs in [2].

Furthermore, we consider a definition of graph which is more general than the one given in most textbooks on graph theory. In particular, we allow edges not to be connected to vertices at both ends. Clearly, all results hold when the number of these *external* edges vanishes and the standard definition of graph is recovered. However, as in [5, 6], external edges are fundamental for the (induction) proofs. This is due to the fact that vertices carrying (labeled) external edges are distinguishable and thus held fixed under any symmetry.

This paper is organized as follows: Section 1 reviews the basic concepts of graph theory that underly much of the paper. Section 2 contains the definitions of the basic linear maps to be used in the following sections. Section 3 translates the recursion formula to generate all connected graphs given in [6], to the language of graph theory. Section 4 extends this result to biconnected, simple and loopless (connected) graphs. The appendixes list all connected graphs (up to three edges), all biconnected graphs (up to four edges), all simple connected graphs (up to five edges), and all loopless connected graphs (up to four edges), with no external edges and together with their scalar factors.

1 Graphs

We briefly review the basic concepts of graph theory that are relevant for the following sections. For more information on these we refer the reader to standard textbooks such as [1].

Let A and B denote sets. By $[A, B]$, we denote the set of all unordered pairs of elements of A and B , $\{a \in A, b \in B\}$. In particular, by $[A]^2 := [A, A]$, we denote the set of all 2-element subsets of A . Also, by 2^A , we denote the power set of A , i.e., the set of all subsets of A . By $\text{card}(A)$, we denote the cardinality of the set A . Finally, we recall that the symmetric difference of the sets A and B is given by $A \triangle B := (A \cup B) \setminus (A \cap B)$.

Let $\mathcal{V} = \{v_i\}_{i \in \mathbb{N}}$ and $\mathcal{K} = \{e_a\}_{a \in \mathbb{N}}$ be infinite sets so that $\mathcal{V} \cap \mathcal{K} = \emptyset$. Let $V \subset \mathcal{V}$; $V \neq \emptyset$ and $K \subset \mathcal{K}$ be finite sets. Let $E = E_{\text{int}} \cup E_{\text{ext}} \subseteq [K]^2$ and $E_{\text{int}} \cap E_{\text{ext}} = \emptyset$. Also, let the

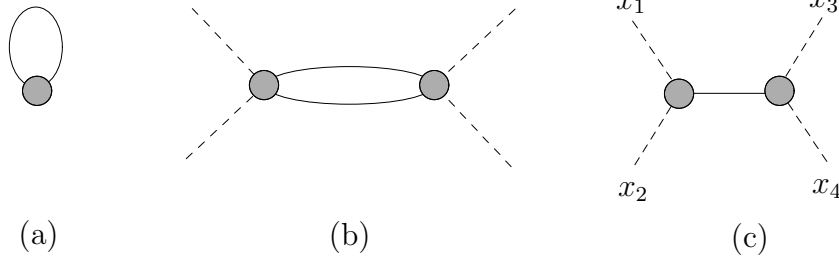


Figure 1: (a) A loop; (b) A graph with both internal and external edges; (c) A graph with labeled external edges. Internal edges are represented by continuous lines, while the external ones are represented by dashed lines.

elements of E satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. In this context, a *graph* is a triple $G = (V, K, E)$ together with the following maps:

(a) $\varphi_{\text{int}} := \eta \circ \zeta : E_{\text{int}} \rightarrow [V]^2 \cup V; \{e_a, e_{a'}\} \mapsto \{v_i, v_{i'}\}$, where

- $\zeta : E_{\text{int}} \rightarrow [K, V] \cup [K]^2; \zeta(\{e_a, e_{a'}\}) = \{e_a, v_{i'}\}$ or $\zeta(\{e_a, e_{a'}\}) = \{e_a, e_{a'}\}$;
- $\eta : [K, V] \cup [K]^2 \rightarrow [V]^2 \cup V; \eta(\{e_a, v_{i'}\}) = \eta(\{e_a, e_{a'}\}) = \{v_i, v_{i'}\}$;

(b) $\varphi_{\text{ext}} : E_{\text{ext}} \rightarrow [V, K]; \{e_a, e_{a'}\} \mapsto \{v_i, e_{a'}\}$.

The elements of V and E are called *vertices* and *edges*, respectively. In particular, the elements of E_{int} and E_{ext} are called *internal* edges and *external* edges, respectively. Both internal and external edges correspond to unordered pairs of elements of K . The elements of these pairs are called *ends* of edges. In other words, internal edges are edges that are connected to vertices at both ends, while external edges have one free end. Internal edges with both ends assigned to the same vertex are also called *loops*. Two distinct vertices connected together by one or more internal edges, are said to be *adjacent*. Two or more internal edges connecting the same pair of distinct vertices together, are called *multiple edges*. For instance, Figure 1 (a) shows a loop, while Figure 1 (b) shows a graph with both multiple edges and external edges. A graph with no loops nor multiple edges is called *simple*. The *degree* of a vertex is the number of ends of edges assigned to the vertex.

Let $G = (V, K, E); E = E_{\text{int}} \cup E_{\text{ext}}, \text{card}(E_{\text{ext}}) = s$, together with the maps φ_{int} and φ_{ext} , denote a graph. The external edges of the graph G are said to be *labeled* if their free ends are assigned labels x_1, \dots, x_s from a *label set* $L = \{x_1, \dots, x_s\}$. Labels on different ends of external edges are required to be distinct. In other words, a *labeling* of the external edges of the graph G , is an injective map $l : E_{\text{ext}} \rightarrow [K, L]; \{e_a, e_{a'}\} \mapsto \{e_a, x_z\}$, where $z \in \{1, \dots, s\}$. For instance, Figure 1 (c) shows a graph with two vertices and four labeled external edges.

A graph $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , is called a *subgraph* of a graph $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} , if $V^* \subseteq V$, $K^* \subseteq K$, $E^* \subseteq E$ and $\varphi_{\text{int}}^* = \varphi_{\text{int}}|_{E_{\text{int}}^*}$, $\varphi_{\text{ext}}^* = \varphi_{\text{ext}}|_{E_{\text{ext}}^*}$.

A *path* is a graph $P = (V, K, E_{\text{int}})$; $V = \{v_1, \dots, v_n\}$, $n := \text{card}(V) > 1$, together with the map φ_{int} , so that $\varphi_{\text{int}}(E_{\text{int}}) = \{\{v_1, v_2\}, \{v_2, v_3\}, \dots, \{v_{n-1}, v_n\}\}$ and the vertices v_1 and v_n have degree 1, while the vertices v_2, \dots, v_{n-1} have degree 2. In this context, the vertices v_1 and v_n are called the *end point* vertices, while the vertices v_2, \dots, v_{n-1} are called the *inner* vertices. A *cycle* is a graph $C = (V', K', E'_{\text{int}})$; $V' = \{v_1, \dots, v_n\}$, together with the map φ'_{int} , so that $\varphi'_{\text{int}}(E'_{\text{int}}) = \{\{v_1, v_2\}, \{v_2, v_3\}, \dots, \{v_{n-1}, v_n\}, \{v_n, v_1\}\}$ and every vertex has degree 2. A graph is said to be *connected* if every pair of vertices is joined by a path. Otherwise, it is *disconnected*. Moreover, a *tree* is a connected graph with no cycles. A *biconnected* graph (or *edge-biconnected* graph) is a connected graph that remains connected after erasing one and whichever internal edge. By definition, a graph consisting of a single vertex is biconnected.

Furthermore, let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph. The set $2^{E_{\text{int}}}$ is a vector space over the field \mathbb{Z}_2 so that vector addition is given by the symmetric difference. The *cycle space* \mathcal{C} of the graph G is defined as the subspace of $2^{E_{\text{int}}}$ generated by all the cycles of G . The dimension of \mathcal{C} is called the *cyclomatic number* of the graph G . Moreover, the cyclomatic number $k := \dim \mathcal{C}$ yields in terms of the vertex number $n := \text{card}(V)$ and the internal edge number $m := \text{card}(E_{\text{int}})$ as $k = m - n + c$, where c denotes the number of connected components of the graph G [4].

Now, let $L = \{x_1, \dots, x_s\}$ be a finite label set. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} , and $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , denote two graphs. Let $l : E_{\text{ext}} \rightarrow [K, L]$ and $l^* : E_{\text{ext}}^* \rightarrow [K^*, L]$ be labelings of the elements of E_{ext} and of E_{ext}^* , respectively. An *isomorphism* between the graphs G and G^* is a bijection $\psi_V : V \rightarrow V^*$ and a bijection $\psi_K : K \rightarrow K^*$ which satisfy the following three conditions:

- (a) If $\varphi_{\text{int}}(\{e_a, e_{a'}\}) = \{v_i, v_{i'}\}$ then $\varphi_{\text{int}}^*(\{\psi_K(e_a), \psi_K(e_{a'})\}) = \{\psi_V(v_i), \psi_V(v_{i'})\}$;
- (b) If $\varphi_{\text{ext}}(\{e_a, e_{a'}\}) = \{v_i, e_{a'}\}$ then $\varphi_{\text{ext}}^*(\{\psi_K(e_a), \psi_K(e_{a'})\}) = \{\psi_V(v_i), \psi_K(e_{a'})\}$;
- (c) $L \cap l(\{e_a, e_{a'}\}) = L \cap l^*(\{\psi_K(e_a), \psi_K(e_{a'})\})$.

Clearly, an isomorphism defines an equivalence relation on graphs. In particular, a *vertex* (resp. *edge*) isomorphism between the graphs G and G^* is an isomorphism so that ψ_E (resp. ψ_V) is the identity map. In this context, a *symmetry* of a graph G , is an isomorphism of the graph onto itself (i.e., an *automorphism*). The order of the group of automorphisms of the graph G is called the *symmetry factor*, denoted by S^G . Also, a *vertex symmetry* (resp. *edge symmetry*) of a graph G , is a vertex (resp. edge) automorphism of the graph. The order of the group of vertex (resp. edge) automorphisms is called the *vertex symmetry factor* (resp. *edge symmetry factor*) of the graph. This is denoted by S_{vertex}^G (resp. S_{edge}^G). Furthermore, the

orders of the groups of vertex and edge automorphisms of a graph G , satisfy $S^G = S_{\text{vertex}}^G \cdot S_{\text{edge}}^G$ (a proof is given in [6], for instance).

2 Elementary linear transformations

We introduce some linear maps and prove their fundamental properties.

Given an arbitrary set W , by $\mathbb{Q}W$, we denote the free vector space on the set W over \mathbb{Q} . That is, (a) every vector in $\mathbb{Q}W$ yields a linear combination of the elements of W with coefficients in \mathbb{Q} ; (b) the set W is linearly independent.

Let $\mathcal{V} = \{v_i\}_{i \in \mathbb{N}}$ and $\mathcal{K} = \{e_a\}_{a \in \mathbb{N}}$ be infinite sets so that $\mathcal{V} \cap \mathcal{K} = \emptyset$. Fix integers $t, s, k \geq 0$ and $n \geq 1$. Let $L = \{x_1, \dots, x_s\}$ be a label set. By $V^{n,k,s}$, we denote the set of all graphs with n vertices, cyclomatic number k and s external edges whose free ends are labeled x_1, \dots, x_s . In all that follows, let $V = \{v_1, \dots, v_n\} \subset \mathcal{V}$, $K = \{e_1, \dots, e_t\} \subset \mathcal{K}$ and $E = E_{\text{int}} \cup E_{\text{ext}}$ be the sets of vertices, of ends of edges and of edges, respectively, of all elements of $V^{n,k,s}$. Also, let $l : E_{\text{ext}} \rightarrow [K, L]$ be a labeling of their external edges. Moreover, by $V_{\text{conn}}^{n,k,s}$ and $V_{\text{disconn}}^{n,k,s}$, we denote the subsets of $V^{n,k,s}$ whose elements are connected or disconnected graphs, respectively. Finally, by $V_{\text{biconn}}^{n,k,s}$, $V_{\text{simple}}^{n,k,s}$ and $V_{\text{loopless}}^{n,k,s}$, we denote the subsets of $V_{\text{conn}}^{n,k,s}$ whose elements are biconnected, simple and loopless graphs, respectively.

We now define the following linear transformations:

- (i) *Assigning a loop to a vertex*: Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$. For all $i \in \{1, \dots, n\}$, define

$$t_i : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k+1,s}; G \mapsto G^*,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfies the following conditions:

- (a) $V^* = V$;
- (b) $K^* = K \cup \{e_{t+1}, e_{t+2}\}$;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}} \cup \{e_{t+1}, e_{t+2}\}$, $E_{\text{ext}}^* = E_{\text{ext}}$;
- (d) $\varphi_{\text{int}}^*|_{E_{\text{int}}} = \varphi_{\text{int}}$ and $\varphi_{\text{int}}^*(\{e_{t+1}, e_{t+2}\}) = \{v_i\}$;
- (e) $\varphi_{\text{ext}}^* = \varphi_{\text{ext}}$.

The t_i -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity. Since the map $t_i : \mathbb{Q}V^{n,k,s} \rightarrow t_i(\mathbb{Q}V^{n,k,s})$ is injective, the operation of *erasing a loop* is given by t_i^{-1} .

- (ii) *Connecting a pair of distinct vertices with an internal edge*: Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$; $n > 1$. For all $i, j \in \{1, \dots, n\}$ with $i \neq j$, define

$$l_{i,j} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k+1,s} \cup \mathbb{Q}V^{n,k,s}; G \mapsto G^*,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfies the following conditions:

- (a) $V^* = V$;
- (b) $K^* = K \cup \{e_{t+1}, e_{t+2}\}$;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}} \cup \{e_{t+1}, e_{t+2}\}$, $E_{\text{ext}}^* = E_{\text{ext}}$;
- (d) $\varphi_{\text{int}}^*|_{E_{\text{int}}} = \varphi_{\text{int}}$ and $\varphi_{\text{int}}^*(\{e_{t+1}, e_{t+2}\}) = \{v_i, v_j\}$;
- (e) $\varphi_{\text{ext}}^* = \varphi_{\text{ext}}$.

The $l_{i,j}$ -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity. Since the map $l_{i,j} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k+1,s}$ is injective, the operation of *erasing an internal edge distinct from a loop* is given by $l_{i,j}^{-1}$. Furthermore, for $n > 1$ (resp. $n > 2$) and for all $i, j \in \{1, \dots, n\}$ with $i \neq j$, define $l_{i,j}^a := l_{i,j} \circ \delta_{i,j}$ (resp. $l_{i,j}^b := l_{i,j} \circ (\text{id} - \delta_{i,j})$), where $\text{id} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k,s}$ is the identity map and $\delta_{i,j} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k,s}; G \mapsto \begin{cases} G & \text{if } \{v_i, v_j\} \in \varphi_{\text{int}}(E_{\text{int}}) \\ 0 & \text{otherwise} \end{cases}$ is a linear map.

- (iii) *Splitting a vertex in two and distributing the ends of edges assigned to the split vertex, between the two new ones in all possible ways*: Let $G = (V, K, E)$ together with the maps $\varphi_{\text{int}} := \eta \circ \zeta$ and φ_{ext} , denote a graph in $V^{n,k,s}$. Let $\mathcal{L}_i \subseteq E$ be the set of edges connected to the vertex $v_i \in V$; $i \in \{1, \dots, n\}$. Also, let $\mathcal{L}_{\text{int},i}$ and $\mathcal{L}_{\text{ext},i}$ be the subsets of \mathcal{L}_i whose elements are internal edges or external edges, respectively. Hence, $\mathcal{L}_i = \mathcal{L}_{\text{int},i} \cup \mathcal{L}_{\text{ext},i}$ and $\mathcal{L}_{\text{int},i} \cap \mathcal{L}_{\text{ext},i} = \emptyset$. Moreover, let $\mathcal{E}_i \subseteq K$ be the set of ends of edges assigned to the vertex v_i . Also, let $\mathcal{E}_{\text{int},i}$ and $\mathcal{E}_{\text{ext},i}$ be the subsets of \mathcal{E}_i whose elements are ends of internal edges or ends of external edges, respectively. Thus, $\mathcal{E}_i = \mathcal{E}_{\text{int},i} \cup \mathcal{E}_{\text{ext},i}$ and $\mathcal{E}_{\text{int},i} \cap \mathcal{E}_{\text{ext},i} = \emptyset$. Let $[\mathcal{E}'_{\text{int},i}]^2 := \mathcal{L}_{\text{int},i} \cap [\mathcal{E}_{\text{int},i}]^2$ and $\mathcal{E}''_{\text{int},i} := \mathcal{E}_{\text{int},i} \setminus \mathcal{E}'_{\text{int},i}$. Finally, let $\mathcal{I}_{\mathcal{E}_i}^2$ denote the set of all partitions of the set \mathcal{E}_i into two disjoint sets: $\mathcal{I}_{\mathcal{E}_i}^2 = \{\{\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}\} : \mathcal{E}_i^{(1)} \cup \mathcal{E}_i^{(2)} = \mathcal{E}_i \text{ and } \mathcal{E}_i^{(1)} \cap \mathcal{E}_i^{(2)} = \emptyset\}$. Clearly, $\mathcal{E}_i^{(b)} = \mathcal{E}_{\text{int},i}^{(b)} \cup \mathcal{E}_{\text{ext},i}^{(b)}$; $b \in \{1, 2\}$. Also, a partition of the set $\mathcal{E}_{\text{ext},i}$, generates a partition of the set $\mathcal{L}_{\text{ext},i}$. Hence, $\mathcal{L}_{\text{ext},i}^{(b)} \subset [\mathcal{E}_{\text{ext},i}^{(b)} K]$. In this context, for all $i \in \{1, \dots, n\}$, define

$$s_{\mathcal{E}_i} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n+1,k-1,s} \cup \mathbb{Q}V^{n+1,k,s}; G \mapsto \sum_{\{\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}\} \in \mathcal{I}_{\mathcal{E}_i}^2} G_{\{\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}\}},$$

where the graphs $G_{\{\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}\}} = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfy the following conditions:

- (a) $V^* = V \cup \{v_{n+1}\}$;
- (b) $K^* = K$;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}}$ and $E_{\text{ext}}^* = E_{\text{ext}}$;
- (d) $\varphi_{\text{int}}^* = \eta^* \circ \zeta^*$, where
 - $\zeta^*|_{E_{\text{int}} \setminus \mathcal{L}_{\text{int},i}} = \zeta|_{E_{\text{int}} \setminus \mathcal{L}_{\text{int},i}}$;
 - $\zeta^*([\mathcal{E}'_{\text{int},i}]^2) = [\mathcal{E}'_{\text{int},i}]^2$;
 - $\zeta^*(\mathcal{L}_{\text{int},i} \setminus [\mathcal{E}'_{\text{int},i}]^2) = [\mathcal{E}''_{\text{int},i}, V']$, where $V' \subseteq V \setminus \{v_i\}$;
 - $\eta^*|_{\zeta(E_{\text{int}} \setminus \mathcal{L}_{\text{int},i})} = \eta|_{\zeta(E_{\text{int}} \setminus \mathcal{L}_{\text{int},i})}$;
 - $\eta^*([\mathcal{E}''_{\text{int},i}, V'] \cup [\mathcal{E}'_{\text{int},i}]^2) = \{v_i\}$ and $\eta^*([\mathcal{E}''_{\text{int},i}, V'] \cup [\mathcal{E}''_{\text{int},i}]^2) = \{v_{n+1}\}$, where $\mathcal{E}''_{\text{int},i} \cup \mathcal{E}''_{\text{int},i} = \mathcal{E}^{(b)}_{\text{int},i}$; $b \in \{1, 2\}$;
- (e) $\varphi_{\text{ext}}^*|_{E_{\text{ext}} \setminus \mathcal{L}_{\text{ext},i}} = \varphi_{\text{ext}}|_{E_{\text{ext}} \setminus \mathcal{L}_{\text{ext},i}}$ and $\varphi_{\text{ext}}^*(\mathcal{L}_{\text{ext},i}^{(1)}) = \{v_i\}$, $\varphi_{\text{ext}}^*(\mathcal{L}_{\text{ext},i}^{(2)}) = \{v_{n+1}\}$.

The $s_{\mathcal{E}_i}$ -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity. Moreover, we define the $s^c_{\mathcal{E}_i}$ -maps (resp. $s^d_{\mathcal{E}_i}$ -maps) by restricting the image of $s_{\mathcal{E}_i}$ to $\mathbb{Q}V_{\text{conn}}^{n+1,k-1,s}$ (resp. $\mathbb{Q}V_{\text{disconn}}^{n+1,k,s}$).

Furthermore, let $l_{i,j}^\rho := \underbrace{l_{i,j} \circ \dots \circ l_{i,j}}_{\rho \text{ times}}$, where ρ is an integer. We now combine the $l_{i,n+1}^\rho$ and $s_{\mathcal{E}_i}$ -maps to define the maps

$$q_i^{(\rho)} := \frac{1}{2(\rho-1)!} l_{i,n+1}^\rho \circ s_{\mathcal{E}_i} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n+1,k+\rho-1,s}.$$

For $\rho = 1$, the definition of $q_i^{(\rho)}$ generalizes the basic operation given in [2] to all partitions of the set \mathcal{E}_i into two sets $\mathcal{E}_i^{(1)}$ and $\mathcal{E}_i^{(2)}$, and to all vertices of the graph. Analogously, the $q_i^{c(\rho)}$ -maps (resp. $q_i^{d(\rho)}$ -maps) are given by the composition of $l_{i,n+1}^\rho$ with $s^c_{\mathcal{E}_i}$ (resp. $s^d_{\mathcal{E}_i}$).

- (iv) In addition, we revise the operation of *contracting an internal edge connecting two distinct vertices, and fusing the two vertices into one* [1]: Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$; $n > 1$. Let $\{e_a, e_{a'}\} \in E_{\text{int}}$ denote an internal edge connecting two distinct vertices, say, $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i < j$. Let $\mathcal{L}_{\text{int},j}$, $\mathcal{L}_{\text{ext},j}$ and $\mathcal{E}_{\text{int},j}$ denote the sets of internal edges, of external edges and of ends of internal edges, respectively, assigned to the vertex v_j . Let $[\mathcal{E}'_{\text{int},j}]^2 :=$

$\mathcal{L}_{\text{int},j} \cap [\mathcal{E}_{\text{int},j}]^2$. Finally, let $[V', v_j] := \varphi_{\text{int}}(\mathcal{L}_{\text{int},j} \setminus [\mathcal{E}'_{\text{int},j}]^2) \subseteq [V \setminus \{v_j\}, v_j]$. In this context, define

$$c_{i,j} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n-1,k,s}; G \mapsto G^*,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfies the following conditions:

- (a) $V^* = \chi_v(V \setminus \{v_j\})$, where $\chi_v : v_l \mapsto \begin{cases} v_l & \forall l \in \{1, \dots, j-1\} \\ v_{l-1} & \forall l \in \{j+1, \dots, n\} \end{cases}$ is a bijection;
- (b) $K^* = \chi_e(K \setminus \{e_a, e_{a'}\})$, where $\chi_e : e_b \mapsto \begin{cases} e_b & \forall b \in \{1, \dots, \min(a, a') - 1\} \\ e_{b-1} & \forall b \in \{\min(a, a') + 1, \dots, \max(a, a') - 1\} \\ e_{b-2} & \forall b \in \{\max(a, a') + 1, \dots, t\} \end{cases}$ is a bijection;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}} \setminus \{e_a, e_{a'}\}$ and $E_{\text{ext}}^* = E_{\text{ext}}$;
- (d) $\varphi_{\text{int}}^*|_{E_{\text{int}}^* \setminus \mathcal{L}_{\text{int},j}} = \varphi_{\text{int}}|_{E_{\text{int}} \setminus \mathcal{L}_{\text{int},j}}$;
 $\varphi_{\text{int}}^*([\mathcal{E}'_{\text{int},j}]^2) = \{v_i\}$, $\varphi_{\text{int}}^*(\mathcal{L}_{\text{int},j} \setminus \{[\mathcal{E}'_{\text{int},j}]^2 \cup \{e_a, e_{a'}\}\}) = [V', v_i]$;
- (e) $\varphi_{\text{ext}}^*|_{E_{\text{ext}} \setminus \mathcal{L}_{\text{ext},j}} = \varphi_{\text{ext}}|_{E_{\text{ext}} \setminus \mathcal{L}_{\text{ext},j}}$ and $\varphi_{\text{ext}}^*(\mathcal{L}_{\text{ext},j}) = \{v_i\}$.

The $c_{i,j}$ -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity.

- (v) *Distributing external edges between all elements of a given subset of vertices in all possible ways*: Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$. Let $V' = \{v_{z_1}, \dots, v_{z_{n'}}\} \subseteq V$; with $1 \leq z_1 < \dots < z_{n'} \leq n$. Let $K' \subset K$ be a finite set so that $K \cap K' = \emptyset$. Also, let $E'_{\text{ext}} \subseteq [K']^2$; $\text{card}(E'_{\text{ext}}) = s'$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Let $L' = \{x_{s+1}, \dots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Also, let $l' : E'_{\text{ext}} \rightarrow [K', L']$ be a labeling of the elements of E'_{ext} . Finally, let $\mathcal{I}_{E'_{\text{ext}}}^{n'}$ denote the set of all partitions of the set E'_{ext} into n' disjoint subsets: $\mathcal{I}_{E'_{\text{ext}}}^{n'} = \{\{E_{\text{ext}}^{(1)}, \dots, E_{\text{ext}}^{(n')}\} : E_{\text{ext}}^{(1)} \cup \dots \cup E_{\text{ext}}^{(n')} = E'_{\text{ext}} \text{ and } E_{\text{ext}}^{(i)} \cap E_{\text{ext}}^{(j)} = \emptyset, \forall i, j \in \{1, \dots, n'\} \text{ with } i \neq j\}$. In this context, define

$$\xi_{E'_{\text{ext}}, V'} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k,s+s'}; G \mapsto \sum_{\{E_{\text{ext}}^{(1)}, \dots, E_{\text{ext}}^{(n')}\} \in \mathcal{I}_{E'_{\text{ext}}}^{n'}} G_{\{E_{\text{ext}}^{(1)}, \dots, E_{\text{ext}}^{(n')}\}},$$

where the graphs $G_{\{E_{\text{ext}}^{(1)}, \dots, E_{\text{ext}}^{(n')}\}} = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfy the following conditions:

- (a) $V^* = V$;
- (b) $K^* = K \cup K'$;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}}$, $E_{\text{ext}}^* = E_{\text{ext}} \cup E'_{\text{ext}}$;

- (d) $\varphi_{\text{int}}^* = \varphi_{\text{int}}$;
- (e) $\varphi_{\text{ext}}^*|_{E_{\text{ext}}} = \varphi_{\text{ext}}$ and $\varphi_{\text{ext}}^*(E_{\text{ext}}^{(i)}) = \{v_{z_i}\}, \forall i \in \{1, \dots, n'\}$;
- (f) $l^* : E_{\text{ext}}^* \rightarrow [K^*, L \cup L']$, with $l^*|_{E_{\text{ext}}} = l$ and $l^*|_{E'_{\text{ext}}} = l'$, is a labeling of the elements of E_{ext}^* .

The $\xi_{E'_{\text{ext}}, V'}$ -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity.

- (vi) *Assigning external edges to vertices which have none:* Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$. Assume that there exists a set $V' \subseteq V$; $\text{card}(V') = s'$ so that $V' \cap \varphi_{\text{ext}}(E_{\text{ext}}) = \emptyset$. Moreover, let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$. Also, let $E'_{\text{ext}} \subseteq [K']^2$; $\text{card}(E'_{\text{ext}}) = s'$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Let $L' = \{x_{s+1}, \dots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Finally, let $l' : E'_{\text{ext}} \rightarrow [K', L']$ be a labeling of the elements of E'_{ext} . In this context, define

$$\epsilon_{E'_{\text{ext}}} : \mathbb{Q}V^{n,k,s} \rightarrow \mathbb{Q}V^{n,k,s+s'}; G \mapsto G^*,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, together with the maps φ_{int}^* and φ_{ext}^* , satisfies the following conditions:

- (a) $V^* = V$;
- (b) $K^* = K \cup K'$;
- (c) $E^* = E_{\text{int}}^* \cup E_{\text{ext}}^*$, where $E_{\text{int}}^* = E_{\text{int}}$, $E_{\text{ext}}^* = E_{\text{ext}} \cup E'_{\text{ext}}$;
- (d) $\varphi_{\text{int}}^* = \varphi_{\text{int}}$;
- (e) $\varphi_{\text{ext}}^*|_{E_{\text{ext}}} = \varphi_{\text{ext}}$ and $\varphi_{\text{ext}}^*(E'_{\text{ext}}) = V'$ is a bijection;
- (f) $l^* : E_{\text{ext}}^* \rightarrow [K^*, L \cup L']$, with $l^*|_{E_{\text{ext}}} = l$ and $l^*|_{E'_{\text{ext}}} = l'$, is a labeling of the elements of E_{ext}^* .

The $\epsilon_{E'_{\text{ext}}}$ -maps are extended to all of $\mathbb{Q}V^{n,k,s}$ by linearity.

The following lemmas are now established.

Lemma 1. *Fix integers $k, s \geq 0$ and $n \geq 1$. Then, for all $i, j \in \{1, \dots, n\}$ with $i \neq j$, the following statements hold:*

- (a) $t_i(\mathbb{Q}V_{\text{conn}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{conn}}^{n,k+1,s}$;
- (b) $l_{i,j}(\mathbb{Q}V_{\text{conn}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{conn}}^{n,k+1,s}$;
- (c) $q_i^{(\rho)}(\mathbb{Q}V_{\text{conn}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{conn}}^{n+1,k+\rho-1,s}$.

Proof. (a), (b) Clearly, the statements hold. (c) Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$. Let \mathcal{E}_i denote the set of ends of edges assigned to the vertex $v_i \in V$. Apply the map $s_{\mathcal{E}_i}$ to the graph G . In particular, $s_{\mathcal{E}_i}(G)$ is a linear combination of graphs, each of which is either connected or disconnected with two components. Applying the $l_{i,n+1}^p$ -map to $s_{\mathcal{E}_i}(G)$ yields connected graphs. This completes the proof. \square

Lemma 2. Fix integers $k, s \geq 0$ and $n \geq 1$. Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$ which is not simple. Then, for all $i, j \in \{1, \dots, n\}$ with $i \neq j$, the following statements hold:

$$(a) \ l_{i,j}^b(G) \notin \mathbb{Q}V_{\text{simple}}^{n,k+1,s};$$

$$(b) \ q_i^{d(1)}(G) \notin \mathbb{Q}V_{\text{simple}}^{n+1,k,s}.$$

Proof. (a) Clearly, the statement holds. (b) For $k = 0$, the statement holds as the $q_i^{d(1)}$ -maps produce trees only from trees. Now, let $n > 1$ and $k > 0$. By assumption, the graph G has at least either one loop or multiple edges. Let \mathcal{E}_i denote the set of ends of edges assigned to the vertex $v_i \in V$. Apply the $s^d_{\mathcal{E}_i}$ -map to graph G . In particular, $s^d_{\mathcal{E}_i}(G)$ is a linear combination of disconnected graphs, each of which is produced from the graph G by assigning all ends of internal edges belonging to the same cycles, from the vertex v_i to either v_i or v_{n+1} . Therefore, at least one of the two components of the graphs in $s^d_{\mathcal{E}_i}(G)$, is not simple. Applying the $l_{i,n+1}$ -map to $s^d_{\mathcal{E}_i}(G)$ cannot produce simple graphs. This completes the proof. \square

Lemma 3. Fix integers $k, s \geq 0$ and $n \geq 1$. Then, for all $i, j \in \{1, \dots, n\}$ with $i \neq j$, the following statements hold:

$$(a) \ l_{i,j}^b(\mathbb{Q}V_{\text{simple}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{simple}}^{n,k+1,s};$$

$$(b) \ q_i^{(1)}(\mathbb{Q}V_{\text{simple}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{simple}}^{n+1,k,s}.$$

Proof. Applying the $l_{i,j}^b$ or $q_i^{(1)}$ -maps to a simple graph cannot introduce loops nor multiple edges. \square

Lemma 4. Fix integers $k, s \geq 0$ and $n \geq 1$. Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V^{n,k,s}$ which is not biconnected. Then, for all $i \in \{1, \dots, n\}$, the following statements hold:

$$(a) \ t_i(G) \notin \mathbb{Q}V_{\text{biconn}}^{n,k+1,s};$$

$$(b) \ q_i^{(1)}(G) \notin \mathbb{Q}V_{\text{biconn}}^{n+1,k,s}.$$

Proof. (a) Clearly, the statement holds. (b) First, by definition all connected graphs with only one vertex are biconnected. Consequently, the $q_i^{(1)}$ -maps produce biconnected graphs with two vertices only from biconnected ones. Now, let $n > 1$. By assumption, the graph G has at least one internal edge which does not belong to any cycle. Therefore, it connects two (distinct) vertices that must be connected together with only one internal edge. Let these vertices be $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i \neq j$, for instance. Apply the $q_i^{(1)}$ -map to the graph G . In particular, $q_i^{(1)}(G)$ is a linear combination of graphs, each of which is so that the vertex v_j is connected with only one internal edge either to v_i or v_{n+1} (but not to both). Clearly, only cycles containing the vertex v_i , are affected by the $q_i^{(1)}$ -map. That is, the vertex v_j cannot share a cycle with neither of the vertices v_i or v_{n+1} . Hence, the graphs in $q_i^{(1)}(G)$ are not biconnected. This completes the proof. \square

Lemma 5. *Fix integers $k, s \geq 0$ and $n \geq 1$. Then, for all $i \in \{1, \dots, n\}$, the following statements hold:*

- (a) $t_i(\mathbb{Q}V_{\text{biconn}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{biconn}}^{n,k+1,s}$;
- (b) $q_i^{c(1)}(\mathbb{Q}V_{\text{biconn}}^{n,k,s}) \subseteq \mathbb{Q}V_{\text{biconn}}^{n+1,k,s}$.

Proof. (a) Clearly, the statement holds. (b) Let $G = (V, K, E)$ together with the maps φ_{int} and φ_{ext} , denote a graph in $V_{\text{biconn}}^{n,k,s}$. Let \mathcal{E}_i denote the set of ends of edges assigned to the vertex $v_i \in V$. Apply the $s^c_{\mathcal{E}_i}$ -map to the graph G . In particular, $s^c_{\mathcal{E}_i}(G)$ is a linear combination of graphs, each of which is produced from the graph G by transforming one or more cycles containing the vertex v_i , into paths whose end point vertices are v_i and v_{n+1} . Moreover, every way to assign the remaining ends of internal edges in the process, from v_i to either v_i or v_{n+1} , defines new cycles. Therefore, applying the $l_{i,n+1}$ -map to $s^c_{\mathcal{E}_i}(G)$, restores the broken cycles and yields biconnected graphs. This completes the proof. \square

3 Arbitrary connected graphs

The present section has substantial overlap with Section II of [6]. Its main result is a recursion formula to generate all connected graphs directly in the algebraic representation rooted in [5]. Here, we formulate that formula on the level of graphs. In a recursion step, the formula yields the linear combination of all graphs having the same vertex and cyclomatic numbers. Moreover, the sum of the coefficients of all graphs in the same equivalence class, corresponds to the inverse of the order of their group of automorphisms. Notice that in [5, 6], the ordering of the vertices is not explicitly taken into account. That is, only one representative of each equivalence class is considered, the coefficient of such graph being given by the sum of the coefficients of all graphs in the same equivalence class.

We use the t_i and $q_i^{(1)}$ -maps defined in the preceding section to recursively generate all connected graphs.

Theorem 6. Fix an integer $s \geq 0$. For all integers $k \geq 0$ and $n \geq 1$, define $\omega^{n,k,s} \in \mathbb{Q}V_{\text{conn}}^{n,k,s}$ by the following recursion relation:

- $\omega^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled x_1, \dots, x_s , and unit coefficient;

•

$$\omega^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{(1)}(\omega^{n-1,k,s}) + \frac{1}{2} \sum_{i=1}^n t_i(\omega^{n,k-1,s}) \right). \quad (1)$$

Then, for fixed values of n and k , $\omega^{n,k,s} = \sum_{G \in V_{\text{conn}}^{n,k,s}} \alpha_G G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$; for all $G \in V_{\text{conn}}^{n,k,s}$. Moreover, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{\text{conn}}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathcal{C}}$ denotes their symmetry factor.

In the recursion equation above, the t_i summand does not appear when $k = 0$. In particular, for $k = 0$, formula (1) specializes to recursively generate all trees. Moreover, formula (1) is an instance of a double recursion. Therefore, its algorithmic implementation is that of any recursive function that makes two calls to itself, such as the defining recurrence of the binomial coefficients.

Proof. The proof is nearly the same to that of Theorem 10 of [6]. The procedure is also very analogous to the one given in [5]. We translate every lemma given in Section II of the former paper to the present setting.

Lemma 7. Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\omega^{n,k,s} = \sum_{G \in V_{\text{conn}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{conn}}^{n,k,s}$ be defined by formula (1). Then, $\alpha_G > 0$ for all $G \in V_{\text{conn}}^{n,k,s}$.

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the result to hold for an arbitrary number of internal edges $m-1$. Let $G = (V, K, E) \in V_{\text{conn}}^{n,k,s}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} , denote a graph. We show that the graph G is generated by applying the t_i -maps to graphs occurring in $\omega^{n,k-1,s} = \sum_{G^* \in V_{\text{conn}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$, or the $q_i^{(1)}$ -maps to graphs occurring in $\omega^{n-1,k,s} = \sum_{G' \in V_{\text{conn}}^{n-1,k,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$:

- Suppose that the graph G has at least one vertex with one or more loops. Let this vertex be $v_i \in V$; $i \in \{1, \dots, n\}$, for instance. Erasing any loop, yields a graph $t_i^{-1}(G) \in \mathbb{Q}V_{\text{conn}}^{n,k-1,s}$. By induction assumption, $\gamma_{t_i^{-1}(G)} > 0$. Hence, applying the t_i -map to the graph $t_i^{-1}(G)$ produces again the graph G . That is, $\alpha_G > 0$.

- (ii) Suppose that the graph G has no loops. There exists $i \in \{1, \dots, n-1\}$ so that $\{v_i, v_n\} \in \varphi_{\text{int}}(E_{\text{int}})$. Applying the $c_{i,n}$ -map to the graph G yields a graph $c_{i,n}(G) \in \mathbb{Q}V_{\text{conn}}^{n-1,k,s}$. By induction assumption, $\beta_{c_{i,n}(G)} > 0$. Hence, applying the $q_i^{(1)}$ -map to the graph $c_{i,n}(G)$, produces a linear combination of graphs, one of which is the graph G . That is, $\alpha_G > 0$.

□

What remains in order to prove Theorem 6 is to show that the sum of the coefficients of all graphs in the same equivalence class, is given by the inverse of their symmetry factor. We start with a more restricted result.

Lemma 8. *Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathcal{C} \subseteq V_{\text{conn}}^{n,k,s}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$ together with the maps φ_{int} and φ_{ext} , denote a graph in \mathcal{C} . Assume that $V \cap \varphi_{\text{ext}}(E_{\text{ext}}) = V$. Let $\omega^{n,k,s} = \sum_{G \in V_{\text{conn}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{conn}}^{n,k,s}$ be defined by formula (1). Then, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $S^{\mathcal{C}}$ denotes the symmetry factor of every graph in \mathcal{C} .*

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general internal edge number $m - 1$. Consider the graph $G = (V, K, E) \in \mathcal{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} . By Lemma 7, the coefficient of the graph G in $\omega^{n,k,s}$ is positive, i.e., $\alpha_G > 0$. We proceed to show that $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$. In particular, the graph $G \in \mathcal{C}$ is so that every one of its vertices has at least one (labeled) external edge. That is, the graph G has no non-trivial vertex symmetries: $S_{\text{vertex}}^{\mathcal{C}} = 1$. Hence, $S^{\mathcal{C}} = S_{\text{edge}}^{\mathcal{C}}$ as any symmetry is an edge symmetry. We check from which graphs with $m - 1$ internal edges, the graphs in the equivalence class \mathcal{C} are generated by the recursion formula (1), and how many times they are generated. To this end, choose any one of the m internal edges of the graph $G \in \mathcal{C}$:

- (i) If that internal edge is a loop, let this be assigned to the vertex $v_i \in V$; $i \in \{1, \dots, n\}$, for instance. Also, assume that the vertex v_i has exactly $1 \leq \tau \leq k$ loops as well as $x \geq 1$ external edges whose free ends are labeled x_{a_1}, \dots, x_{a_x} , with $1 \leq a_1 < \dots < a_x \leq s$. Erasing any one of these loops yields a graph $t_i^{-1}(G)$ whose symmetry factor is related to that of $G \in \mathcal{C}$ via $S^{t_i^{-1}(G)} = S^{\mathcal{C}}/(2\tau)$. Let $\omega^{n,k-1,s} = \sum_{G^* \in V_{\text{conn}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathcal{A} \subseteq V_{\text{conn}}^{n,k-1,s}$ denote the equivalence class containing $t_i^{-1}(G)$. The t_i -map produces the graph G from the graph $t_i^{-1}(G)$ with coefficient $\alpha_G^* = \gamma_{t_i^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph $t_i^{-1}(G)$ has at least one labeled external edge. Hence, by induction assumption, $\sum_{G^* \in \mathcal{A}} \gamma_{G^*} = 1/S^{t_i^{-1}(G)} = 1/S^{\mathcal{A}}$. Now, take one graph (distinct from the graph G) in \mathcal{C} in turn, choose one of the loops of the vertex having x external edges whose free ends are labeled x_{a_1}, \dots, x_{a_x} , and repeat the procedure above. We obtain

$$\sum_{G \in \mathcal{C}} \alpha_G^* = \sum_{G^* \in \mathcal{A}} \gamma_{G^*} = \frac{1}{S^{\mathcal{A}}} = \frac{2\tau}{S^{\mathcal{C}}}.$$

Therefore, the contribution to $\sum_{G \in \mathcal{C}} \alpha_G$ is $\tau/(m \cdot S^{\mathcal{C}})$. Distributing this factor between the τ loops considered yields $1/(m \cdot S^{\mathcal{C}})$ for each loop.

- (ii) If that internal edge is not a loop, let this be connected to the vertices, $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i < j$, for instance. Also, assume that v_i has $\tau' \geq 0$ loops as well as $r \geq 1$ external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , with $1 \leq a_1 < \dots < a_r \leq s$, while v_j has $\tau'' \geq 0$ loops as well as $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, with $1 \leq b_1 < \dots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \dots, r\}, z' \in \{1, \dots, r'\}$. Finally, assume that the two vertices are connected together with $\rho \geq 1$ internal edges, so that $1 \leq \tau' + \tau'' + \rho \leq k + 1$. Contracting any one of these internal edges, yields a graph $c_{i,j}(G)$ whose i th vertex, has $\mu := \tau' + \tau'' + \rho - 1$ loops as well as $r + r'$ external edges whose free ends are labeled $x_{a_1}, \dots, x_{a_r}, x_{b_1}, \dots, x_{b_{r'}}$. Consequently, the symmetry factor of the graph $c_{i,j}(G)$ is related to that of $G \in \mathcal{C}$ via

$$\frac{1}{2^\mu} \frac{1}{\mu!} S^{c_{i,j}(G)} = \frac{1}{2^{\tau'} \tau'!} \frac{1}{2^{\tau''} \tau''!} \frac{1}{\rho!} S^{\mathcal{C}}.$$

Let $\omega^{n-1,k,s} = \sum_{G' \in V_{\text{conn}}^{n-1,k,s}} \beta_{G'} G'; \beta_{G'} \in \mathbb{Q}$. Let $\mathcal{B} \subseteq V_{\text{conn}}^{n-1,k,s}$ denote the equivalence class containing $c_{i,j}(G)$. Applying the $q_i^{(1)}$ -map to $c_{i,j}(G)$ yields a linear combination of graphs, one of which, is isomorphic to the graph G . To calculate the coefficient $\alpha'_G \in \mathbb{Q}$ of such graph in that linear combination, we need to count the number of different ways to distribute the $2\mu + r + r'$ ends of edges assigned to the vertex v_i , between the two new ones, so that one vertex is assigned with r external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , as well as τ' loops, the other is assigned with r' external edges whose free ends are labeled by $x_{b_1}, \dots, x_{b_{r'}}$, as well as τ'' loops, while the remaining $\rho - 1$ internal edges are employed to connect the two vertices together. Now, there are two ways to assign the given r external edges to one vertex and the given r' external edges to the other. Moreover, there are $\binom{\mu}{\tau'} = \frac{\mu!}{(\mu - \tau')! \tau'!}$ ways to assign both ends of τ' internal edges chosen among the μ internal edges in the process, to the vertex with the aforesaid r external edges. Besides, there are $\binom{\mu - \tau'}{\tau''} = \frac{(\mu - \tau')!}{(\mu - \tau' - \tau'')! \tau''!}$ ways to assign both ends of τ'' internal edges chosen among the $\mu - \tau'$ internal edges in the process, to the vertex with the aforesaid r' external edges. Finally, there are two ways to distribute one end of each of the remaining $\rho - 1$ internal edges, per vertex. This yields $2^{\rho-1}$ ways to connect the two new vertices together with $\rho - 1$ internal edges. The final result is given by the product of all these factors. Hence, there are

$$2 \cdot 2^{\rho-1} \frac{\mu!}{(\mu - \tau')! \tau'!} \cdot \frac{(\mu - \tau')!}{(\mu - \tau' - \tau'')! \tau''!} = 2^\rho \frac{\mu!}{\tau'! \tau''! (\rho - 1)!}$$

ways to distribute the $2\mu + r + r'$ ends of edges between the two new vertices in order to produce a graph in the equivalence class \mathcal{C} . Hence, $\alpha'_G = 2^{\rho-1} \frac{\mu!}{\tau'! \tau''! (\rho-1)!} \beta_{c_{i,j}(G)}$. Each

vertex of the graph $c_{i,j}(G)$ has at least one labeled external edge. Thus, by induction assumption, $\sum_{G' \in \mathcal{B}} \beta_{G'} = 1/S^{c_{i,j}(G)} = 1/S^{\mathcal{B}}$. Now, take one graph (distinct from G) in \mathcal{C} in turn, choose one of the internal edges connecting together the pair of vertices so that one vertex has r external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , while the other has r' external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\begin{aligned} \sum_{G \in \mathcal{C}} \alpha'_G &= 2^{\rho-1} \frac{\mu!}{\tau'! \tau''! (\rho-1)!} \sum_{G' \in \mathcal{B}} \beta_{G'} \\ &= 2^{\rho-1} \frac{\mu!}{\tau'! \tau''! (\rho-1)!} \frac{1}{S^{\mathcal{B}}} \\ &= 2^{\rho-1} \frac{\mu!}{\tau'! \tau''! (\rho-1)!} \cdot \frac{\tau'! \tau''! \rho!}{\mu!} \cdot \frac{1}{2^{\rho-1} S^{\mathcal{C}}} \\ &= \frac{\rho}{S^{\mathcal{C}}}. \end{aligned}$$

Therefore, the contribution to $\sum_{G \in \mathcal{C}} \alpha_G$ is $\rho/(m \cdot S^{\mathcal{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m \cdot S^{\mathcal{C}})$ for each edge.

We conclude that every one of the m internal edges of the graph G contributes with a factor of $1/(m \cdot S^{\mathcal{C}})$ to $\sum_{G \in \mathcal{C}} \alpha_G$. Hence, the overall contribution is exactly $1/S^{\mathcal{C}}$. This completes the proof. \square

$\omega^{k,n,n}$ satisfies the following property:

Lemma 9. *Fix integers $k, s \geq 0$ and $n \geq 1$. Let $\omega^{n,k,s} = \sum_{G \in V_{\text{conn}}^{n,k,s}} \alpha_G$ $G \in \mathbb{Q}V_{\text{conn}}^{n,k,s}$ be defined by formula (1). Let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$. Let $E'_{\text{ext}} \subseteq [K']^2$; $\text{card}(E'_{\text{ext}}) = s'$. Also, assume that the elements of E'_{ext} satisfy $\{e_b, e_{b'}\} \cap \{e_c, e_{c'}\} = \emptyset$. Let $L' = \{x_{s+1}, \dots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Let $l' : E'_{\text{ext}} \rightarrow [K', L']$ be a labeling of the elements of E'_{ext} . Then, $\omega^{n,k,s+s'} = \xi_{E'_{\text{ext}}, V}(\omega^{n,k,s})$.*

Proof. Let $E_{\text{ext}}^* := E_{\text{ext}} \cup E'_{\text{ext}}$ be the set of external edges of all graphs occurring in $\omega^{n-1,k,s+s'} \in \mathbb{Q}V_{\text{conn}}^{n-1,k,s+s'}$. Let $V' = \{v_1, \dots, v_{n-1}\}$ be their vertex set. Let \mathcal{E}_i be the set of ends of edges assigned to the vertex $v_i \in V'$; $i \in \{1, \dots, n-1\}$. Let $\mathcal{E}_{\text{ext},i}$ be the subset of \mathcal{E}_i whose elements are ends of external edges. Also, let $\mathcal{L}_{\text{ext},i}$ be the set of external edges assigned to the vertex v_i . Finally, let $\mathcal{L}_{\text{ext},i}^* := E'_{\text{ext}} \cap \mathcal{L}_{\text{ext},i}$; $\text{card}(\mathcal{L}_{\text{ext},i}^*) = s^*$, and $\mathcal{E}_{\text{ext},i}^* := \mathcal{E}_{\text{ext},i} \cap \mathcal{L}_{\text{ext},i}^*$. In this context, for all $i \in \{1, \dots, n-1\}$, the $s_{\mathcal{E}_i}$ -maps yield as $s_{\mathcal{E}_i} = \xi_{\mathcal{L}_{\text{ext},i}^*, \{v_i, v_n\}} \circ s'_{\mathcal{E}_i \setminus \mathcal{E}_{\text{ext},i}^*}$, where the maps $s'_{\mathcal{E}_i \setminus \mathcal{E}_{\text{ext},i}^*} : \mathbb{Q}V_{\text{conn}}^{n-1,k,s+s'} \rightarrow \mathbb{Q}V^{n,k-1,s+s'-s^*} \cup \mathbb{Q}V^{n,k,s+s'-s^*}$ are required to produce graphs with external edge set $E_{\text{ext}}^* \setminus \mathcal{L}_{\text{ext},i}^*$, from graphs with external edge set E_{ext}^* . Clearly,

$\xi_{E'_{\text{ext}}, V} = \xi_{\mathcal{L}_{\text{ext}, i}^*, \{v_i, v_n\}} \circ \xi_{E'_{\text{ext}} \setminus \mathcal{L}_{\text{ext}, i}^*, V \setminus \{v_i, v_n\}}$. Hence, the equality $\omega^{n, k, s+s'} = \xi_{E'_{\text{ext}}, V}(\omega^{n, k, s})$ follows immediately from the recursive definition (1). \square

We now proceed to show that $\sum_{G \in V_{\text{conn}}^{n, k, s}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{\text{conn}}^{n, k, s}$ denotes any equivalence class.

Lemma 10. *Fix integers $k \geq 0$ and $n \geq 1$. Let $\mathcal{C} \subseteq V_{\text{conn}}^{n, k, s}$ denote an arbitrary equivalence class. Let $\omega^{n, k, s} = \sum_{G \in V_{\text{conn}}^{n, k, s}} \alpha_G G \in \mathbb{Q}V_{\text{conn}}^{n, k, s}$ be defined by formula (1). Then, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $S^{\mathcal{C}}$ denotes the symmetry factor of every graph in \mathcal{C} .*

Proof. Choose a graph $G = (V, K, E) \in \mathcal{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} . If $\varphi_{\text{ext}}(E_{\text{ext}}) = V$, we simply recall Lemma 8. Thus, we may now assume that there exists a set $V' \subseteq V$; $\text{card}(V') = s'$ so that $V' \cap \varphi_{\text{ext}}(E_{\text{ext}}) = \emptyset$. Let $K' \subset K$ be a finite set so that $K \cap K' = \emptyset$. Also, let $E'_{\text{ext}} \subseteq [K']^2$; $\text{card}(E'_{\text{ext}}) = s'$. Assume that the elements of E'_{ext} satisfy $\{e_b, e_{b'}\} \cap \{e_c, e_{c'}\} = \emptyset$. Also, let $L' = \{x_{s+1}, \dots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Finally, let $l' : E'_{\text{ext}} \rightarrow [K', L']$ be a labeling of the elements of E'_{ext} . Now, apply an $\epsilon_{E'_{\text{ext}}}$ -map to the graph G . Let $\mathcal{D} \subseteq V_{\text{conn}}^{n, k, s+s'}$ denote the equivalence class containing $\epsilon_{E'_{\text{ext}}}(G)$. Let $\omega^{n, k, s+s'} = \sum_{G' \in V_{\text{conn}}^{n, k, s+s'}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$. By Lemma 8, $\sum_{G' \in \mathcal{D}} \beta_{G'} = 1/S^{\epsilon_{E'_{\text{ext}}}(G)} = 1/S^{\mathcal{D}}$. Since, in general, the $\epsilon_{E'_{\text{ext}}}$ -maps are not uniquely defined, assume that there are T distinct maps $\epsilon_{E'_{\text{ext}}}^{(l)}$, $l \in \{1, \dots, T\}$ so that $\epsilon_{E'_{\text{ext}}}^{(l)}(G) \in \mathcal{D}$. Clearly, $\beta_{\epsilon_{E'_{\text{ext}}}^{(l)}(G)} = \alpha_G > 0$. Therefore, by repeating the same procedure for every graph in \mathcal{C} and recalling Lemma 9, we obtain

$$\sum_{G' \in \mathcal{D}} \beta_{G'} = \sum_{l=1}^T \sum_{G \in \mathcal{C}} \beta_{\epsilon_{E'_{\text{ext}}}^{(l)}(G)} = T \sum_{G \in \mathcal{C}} \alpha_G = \frac{1}{S^{\mathcal{D}}}.$$

That is, $\sum_{G \in \mathcal{C}} \alpha_G = 1/(T \cdot S^{\mathcal{D}})$. Now, every map $\epsilon_{E'_{\text{ext}}}^{(l)}$ defines a vertex symmetry of the graph G . This can have no more than these vertex symmetries, since the vertices that already carry (labeled) external edges, are distinguishable and thus held fixed under any symmetry. Hence, $S_{\text{vertex}}^G = S_{\text{vertex}}^{\mathcal{C}} = T$. Moreover, $S^{\mathcal{D}} = S_{\text{edge}}^{\mathcal{D}} = S_{\text{edge}}^{\mathcal{C}}$. Finally, from the identity $S^{\mathcal{C}} = S_{\text{vertex}}^{\mathcal{C}} \cdot S_{\text{edge}}^{\mathcal{C}}$, follows that $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$. \square

\square

Appendix A shows the result of computing all mutually non isomorphic connected graphs without external edges as contributions to $\omega^{n, k, 0}$, for internal edge number $m = k + n - 1 \leq 3$.

4 Extensions

We generalize the recursion formula (1) to biconnected, simple and loopless connected graphs. These three results were not obtained in previous papers, using the Hopf algebraic approach given in [5, 6].

4.1 Biconnected graphs

By Lemmas 4 and 5, Theorem 6 specializes to biconnected graphs by replacing the $q_i^{(1)}$ -maps by the $q_i^{c(1)}$ -maps in formula (1).

Theorem 11. *Fix an integer $s \geq 0$. For all integers $k \geq 0$ and $n \geq 1$, define $\beta^{n,k,s} \in \mathbb{Q}V_{biconn}^{n,k,s}$ by the following recursion relation:*

- $\beta^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled x_1, \dots, x_s , and unit coefficient;

•

$$\beta^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{c(1)}(\beta^{n-1,k,s}) + \frac{1}{2} \sum_{i=1}^n t_i(\beta^{n,k-1,s}) \right), k > 0. \quad (2)$$

Then, for fixed values of n and k , $\beta^{n,k,s} = \sum_{G \in V_{biconn}^{n,k,s}} \alpha_G G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$; $\forall G \in V_{biconn}^{n,k,s}$. Moreover, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{biconn}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathcal{C}}$ denotes their symmetry factor.

For $k = 1$ and $n > 1$, formula (2) specializes to recursively generate a cycle with n vertices, s external edges whose free ends are labeled x_1, \dots, x_s , and coefficient $1/(2n)$, from a cycle with $n-1$ vertices, the given external edges and coefficient $1/(2(n-1))$.

Appendix B shows the result of computing all mutually non isomorphic biconnected graphs without external edges as contributions to $\beta^{n,k,0}$, for internal edge number $m = k+n-1 \leq 4$.

4.2 Simple connected graphs

We generalize Theorem 6 to simple connected graphs. To this end, we combine the $q_i^{d(1)}$ -maps with the $l_{i,j}^b$ -maps in formula (1).

Theorem 12. *Fix an integer $s \geq 0$. For all integers $k \geq 0$ and $n \geq 1$, define $\sigma^{n,k,s} \in \mathbb{Q}V_{simple}^{n,k,s}$ by the following recursion relation:*

- $\sigma^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled x_1, \dots, x_s , and unit coefficient;

$$\sigma^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{d(1)}(\sigma^{n-1,k,s}) + \sum_{i=1}^n \sum_{j=1}^{i-1} l_{i,j}^b(\sigma^{n,k-1,s}) \right), n > 1. \quad (3)$$

Then, for fixed values of n and k , $\sigma^{n,k,s} = \sum_{G \in V_{\text{simple}}^{n,k,s}} \alpha_G G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$; for all $G \in V_{\text{simple}}^{n,k,s}$. Moreover, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{\text{simple}}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathcal{C}}$ denotes their symmetry factor.

In the recursion equation above, the $l_{i,j}^b$ summand does not appear when $k = 0$ and/or $n = 2$.

Proof. The proof is very analogous to that of Theorem 6. Actually, every lemma given in the preceding section remains valid by replacing $\omega^{n,k,s}$ by $\sigma^{n,k,s}$. Here, we only state and prove the two lemmas corresponding to Lemmas 7 and 8. The rest of the proof is implied by analogy.

Lemma 13. Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\sigma^{n,k,s} = \sum_{G \in V_{\text{simple}}^{n,k,s}} \alpha_G G \in \mathbb{Q} V_{\text{simple}}^{n,k,s}$ be defined by formula (3). Then, $\alpha_G > 0$ for all $G \in V_{\text{simple}}^{n,k,s}$.

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the result to hold for an arbitrary internal edge number $m - 1$. Let $G = (V, K, E) \in V_{\text{simple}}^{n,k,s}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} , denote a graph. We show that the graph G is generated by applying the $l_{i,j}^b$ -maps to graphs occurring in $\sigma^{n,k-1,s} = \sum_{G^* \in V_{\text{simple}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$, or the $q_i^{d(1)}$ -maps to graphs occurring in $\sigma^{n-1,k,s} = \sum_{G' \in V_{\text{simple}}^{n-1,k,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$:

- (i) If $k = 0$, by Lemma 7, $\alpha_G > 0$.
- (ii) If $k > 0$, choose any one of the internal edges of the graph G which belong at least to one cycle. Let this be connected to the vertices v_i, v_j ; $i, j \in \{1, \dots, n\}$ with $i \neq j$, for instance. Erasing such internal edge, yields a graph $l_{i,j}^{-1}(G) \in \mathbb{Q} V_{\text{simple}}^{n,k-1,s}$. By induction assumption, $\gamma_{l_{i,j}^{-1}(G)} > 0$. Hence, applying the $l_{i,j}^b$ -map to $l_{i,j}^{-1}(G)$ produces again the graph G . That is, $\alpha_G > 0$.

□

Lemma 14. Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathcal{C} \subseteq V_{\text{simple}}^{n,k,s}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} , denote a graph in \mathcal{C} . Assume that $V \cap \varphi_{\text{ext}}(E_{\text{ext}}) = V$. Let $\sigma^{n,k,s} = \sum_{G \in V_{\text{simple}}^{n,k,s}} \alpha_G G \in \mathbb{Q} V_{\text{simple}}^{n,k,s}$ be defined by formula (3). Then, $\sum_{G \in \mathcal{C}} \alpha_G = 1$.

Proof. The proof proceeds by induction on the internal edge number: $m = k + n - 1$. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general internal edge number $m - 1$. Consider the graph $G = (V, K, E) \in \mathcal{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} . By Lemma 13, the coefficient of the graph $G \in \mathcal{C}$ is positive: $\alpha_G > 0$. In particular, $S^{\mathcal{C}} = 1$ as the graph G is simple and every one of its vertices has at least one external edge. We proceed to show that $\sum_{G \in \mathcal{C}} \alpha_G = 1$. To this end, choose any one of the m internal edges of the graph $G \in \mathcal{C}$:

- (i) If that internal edge does not belong to any cycle, by Lemma 8, it contributes with a factor of $1/m$ to $\sum_{G \in \mathcal{C}} \alpha_G$.
- (ii) If that internal edge belongs at least to one cycle, let this be connected to the vertices $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i \neq j$, for instance. Also, assume that v_i has $r \geq 1$ external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , with $1 \leq a_1 < \dots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, with $1 \leq b_1 < \dots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \dots, r\}, z' \in \{1, \dots, r'\}$. Erasing the given internal edge yields a graph $l_{i,j}^{-1}(G)$ so that $S^{l_{i,j}^{-1}(G)} = 1$. Let $\sigma^{n,k-1,s} = \sum_{G^* \in V_{\text{simple}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathcal{A} \subseteq V_{\text{simple}}^{n,k-1,s}$ denote the equivalence class containing $l_{i,j}^{-1}(G)$. The $l_{i,j}^b$ -map produces the graph G from the graph $l_{i,j}^{-1}(G)$ with coefficient $\alpha_G^* = \gamma_{l_{i,j}^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph $l_{i,j}^{-1}(G)$ has at least one labeled external edge. Hence, by induction assumption, $\sum_{G^* \in \mathcal{A}} \gamma_{G^*} = 1$. Now, take one graph (distinct from G) in \mathcal{C} in turn, choose the internal edge connected to the vertex having r external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , and to the vertex having r' external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\sum_{G \in \mathcal{C}} \alpha_G^* = \sum_{G^* \in \mathcal{A}} \gamma_{G^*} = 1.$$

Therefore, the contribution to $\sum_{G \in \mathcal{C}} \alpha_G$ is $1/m$.

We conclude that every one of the m internal edges of the graph G contributes with a factor of $1/m$ to $\sum_{G \in \mathcal{C}} \alpha_G$. Hence, the overall contribution is exactly 1. This completes the proof. \square

\square

Appendix C shows the result of computing all mutually non isomorphic simple connected graphs without external edges as contributions to $\sigma^{n,k,0}$, for internal edge number $m = k + n - 1 \leq 5$.

4.3 Loopless connected graphs

The present section presents two algorithms to generate all loopless connected graphs. The second one is amenable for direct implementation via Hopf algebras in the sense of [5, 6].

4.3.1 Main recursion formula

We generalize Theorem 6 to loopless connected graphs. To this end, we replace the t_i -maps by the $l^a_{i,j}$ -maps in formula (1).

Theorem 15. *Fix an integer $s \geq 0$. For all integers $k \geq 0$ and $n \geq 1$, define $\theta^{n,k,s} \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ by the following recursion relation:*

- $\theta^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled x_1, \dots, x_s , and unit coefficient;

•

$$\theta^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{(1)}(\theta^{n-1,k,s}) + \sum_{i=1}^n \sum_{j=1}^{i-1} l^a_{i,j}(\theta^{n,k-1,s}) \right), n > 1. \quad (4)$$

Then, for fixed values of n and k , $\theta^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V_{\text{loopless}}^{n,k,s}$. Moreover, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{\text{loopless}}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathcal{C}}$ denotes their symmetry factor.

In the recursion equation above, the $l^a_{i,j}$ summand does not appear when $k = 0$.

Proof. As in the preceding section, every lemma given in Section 3 holds when stated for $\theta^{n,k,s}$. Hence, we restrict the proof of Theorem 15 to the following two lemmas.

Lemma 16. *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\theta^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ be defined by formula (4). Then, $\alpha_G > 0$ for all $G \in V_{\text{loopless}}^{n,k,s}$.*

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the result to hold for an arbitrary internal edge number $m - 1$. Let $G = (V, K, E) \in V_{\text{loopless}}^{n,k,s}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} , denote a graph. We show that the graph G is generated by applying the $l^a_{i,j}$ -maps to graphs occurring in $\theta^{n,k-1,s} = \sum_{G^* \in V_{\text{loopless}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$, or the $q_i^{(1)}$ -maps to graphs occurring in $\theta^{n-1,k,s} = \sum_{G' \in V_{\text{loopless}}^{n-1,k,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$:

- Suppose that the graph G has no multiple edges. By Lemma 7, $\alpha_G > 0$.

- (ii) Suppose that the graph G has at least one pair of vertices, say, $v_i, v_j \in V; i, j \in \{1, \dots, n\}$ with $i \neq j$, connected together by multiple edges. Erasing any one of those edges, yields a graph $l_{i,j}^{-1}(G) \in \mathbb{Q}V_{\text{loopless}}^{n,k-1,s}$. By induction assumption, $\gamma_{l_{i,j}^{-1}(G)} > 0$. Hence, applying the $l_{i,j}^a$ -map to $l_{i,j}^{-1}(G)$ produces again the graph G . That is, $\alpha_G > 0$.

□

Lemma 17. Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathcal{C} \subseteq V_{\text{loopless}}^{n,k,s}$ denote an equivalence class. Let $G = (V, K, E); E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} , denote a graph in \mathcal{C} . Assume that $V \cap \varphi_{\text{ext}}(E_{\text{ext}}) = V$. Let $\theta^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ be defined by formula (4). Then, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $S^{\mathcal{C}}$ denotes the symmetry factor of every graph in \mathcal{C} .

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m - 1$. Consider the graph $G = (V, K, E) \in \mathcal{C}; E = E_{\text{int}} \cup E_{\text{ext}}, m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} . By Lemma 16, the coefficient of the graph $G \in \mathcal{C}$ is positive: $\alpha_G > 0$. We proceed to show that $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$. To this end, choose any one of the m internal edges of the graph $G \in \mathcal{C}$:

- (i) If that internal edge is the only one connecting a given pair of vertices together, by Lemma 8, it contributes with a factor of $1/(m \cdot S^{\mathcal{C}})$ to $\sum_{G \in \mathcal{C}} \alpha_G$.
- (ii) If that internal edge is one of the, say, $1 < \rho \leq k + 1$, multiple edges connecting together the vertices $v_i, v_j \in V; i, j \in \{1, \dots, n\}$ with $i \neq j$, for instance, assume that v_i has $r \geq 1$ external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , with $1 \leq a_1 < \dots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, with $1 \leq b_1 < \dots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \dots, r\}, z' \in \{1, \dots, r'\}$. Erasing any one of the given internal edges yields a graph $l_{i,j}^{-1}(G)$ whose symmetry factor is related to that of the graph $G \in \mathcal{C}$ via $S^{l_{i,j}^{-1}(G)} = S^{\mathcal{C}}/\rho$. Let $\theta^{n,k-1,s} = \sum_{G^* \in V_{\text{loopless}}^{n,k-1,s}} \gamma_{G^*} G^*; \gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathcal{A} \subseteq V_{\text{loopless}}^{n,k-1,s}$ denote the equivalence class containing $l_{i,j}^{-1}(G)$. The $l_{i,j}^a$ -map produces the graph G from the graph $l_{i,j}^{-1}(G)$ with coefficient $\alpha_G^* = \gamma_{l_{i,j}^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph $l_{i,j}^{-1}(G)$ has at least one labeled external edge. Hence, by induction assumption, $\sum_{G^* \in \mathcal{A}} \gamma_{G^*} = 1/S^{l_{i,j}^{-1}(G)} = 1/S^{\mathcal{A}}$. Now, take one graph (distinct from G) in \mathcal{C} in turn, choose one of the internal edges connecting together the pair of vertices so that one vertex has r external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , while the other has r' external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, and repeat the

procedure above. We obtain

$$\sum_{G \in \mathcal{C}} \alpha_G^* = \sum_{G \in \mathcal{A}} \gamma_{G^*} = \frac{1}{S^{\mathcal{A}}} = \frac{\rho}{S^{\mathcal{C}}}.$$

Therefore, the contribution to $\sum_{G \in \mathcal{C}} \alpha_G$ is $\rho/(m \cdot S^{\mathcal{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m \cdot S^{\mathcal{C}})$ for each internal edge.

We conclude that every one of the m internal edges of the graph G contributes with a factor of $1/(m \cdot S^{\mathcal{C}})$ to $\sum_{G \in \mathcal{C}} \alpha_G$. Hence, the overall contribution is exactly $1/S^{\mathcal{C}}$. This completes the proof. \square

\square

4.3.2 Alternative recursion formula

We present an alternative recursion formula for loopless connected graphs. The underlying algorithm is amenable to direct implementation using the algebraic representation of graphs given in [5, 6].

Theorem 18. *Fix an integer $s \geq 0$. For all integers $k \geq 0$ and $n \geq 1$, define $\hat{\theta}^{n,k,s} \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ by the following recursion relation:*

- $\hat{\theta}^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled x_1, \dots, x_s , and unit coefficient;
- $\hat{\theta}^{1,k,s} := 0$, $k > 0$;
-

$$\hat{\theta}^{n,k,s} := \frac{1}{k+n-1} \sum_{\rho=1}^{k+1} \sum_{i=1}^{n-1} q_i^{(\rho)} (\hat{\theta}^{n-1,k+1-\rho,s}), n > 1. \quad (5)$$

Then, for fixed values of n and k , $\hat{\theta}^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$; for all $G \in V_{\text{loopless}}^{n,k,s}$. Moreover, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $\mathcal{C} \subseteq V_{\text{loopless}}^{n,k,s}$ denotes an arbitrary equivalence of graphs class of graphs and $S^{\mathcal{C}}$ denotes their symmetry factor.

Proof. As in the previous sections, every lemma given in Section 3 holds for $\hat{\theta}^{n,k,s}$. Here, details are only given for the following two lemmas.

Lemma 19. *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\hat{\theta}^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ be defined by formula (5). Then, $\alpha_G > 0$ for all $G \in V_{\text{loopless}}^{n,k,s}$.*

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the statement to hold for any internal edge number smaller than a fixed $m \geq 1$. Let $G = (V, K, E) \in V_{\text{loopless}}^{n,k,s}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} , denote a graph. We show that the graph G is generated by applying the $q_i^{(\rho)}$ -maps to graphs occurring in $\hat{\theta}^{n-1,k+1-\rho,s} = \sum_{G' \in V_{\text{loopless}}^{n-1,k+1-\rho,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$: There exists $i \in \{1, \dots, n-1\}$ so that $\{v_i, v_n\} \in \varphi_{\text{int}}(E_{\text{int}})$. Assume that the two vertices are connected together with $1 \leq \rho \leq k+1$ internal edges. Applying the map $c_{i,n} \circ l_{i,n}^{1-\rho}$ to the graph G yields a graph $G' := (c_{i,n} \circ l_{i,n}^{1-\rho})(G) \in \mathbb{Q}V_{\text{loopless}}^{n-1,k-\rho+1,s}$. By induction assumption, $\beta_{G'} > 0$. Hence, applying the $q_i^{(\rho)}$ -map to the graph G' , produces a linear combination of graphs, one of which is the graph G . That is, $\alpha_G > 0$. This completes the proof. \square

Lemma 20. Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathcal{C} \subseteq V_{\text{loopless}}^{n,k,s}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} , denote a graph in \mathcal{C} . Assume that $V \cap \varphi_{\text{ext}}(E_{\text{ext}}) = V$. Let $\hat{\theta}^{n,k,s} = \sum_{G \in V_{\text{loopless}}^{n,k,s}} \alpha_G G \in \mathbb{Q}V_{\text{loopless}}^{n,k,s}$ be defined by formula (5). Then, $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$, where $S^{\mathcal{C}}$ denotes the symmetry factor of every graph in \mathcal{C} .

Proof. The proof proceeds by induction on the internal edge number m . Clearly, the statement holds for $m = 0$. We assume the statement to hold for any internal edge number smaller than a fixed $m \geq 1$. Consider the graph $G = (V, K, E) \in \mathcal{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$; $m = \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext} . By Lemma 19, the coefficient of the graph $G \in \mathcal{C}$ is positive: $\alpha_G > 0$. We proceed to show that $\sum_{G \in \mathcal{C}} \alpha_G = 1/S^{\mathcal{C}}$: Choose any one of the m internal edges of the graph $G \in \mathcal{C}$. Let this be connected to the vertices $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i < j$, for instance. Also, assume that v_i has $r \geq 1$ external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , with $1 \leq a_1 < \dots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \dots, x_{b_{r'}}$, with $1 \leq b_1 < \dots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \dots, r\}, z' \in \{1, \dots, r'\}$. Finally, assume that there are $1 \leq \rho \leq k+1$ multiple edges connecting the vertices v_i and v_j together. Erasing $\rho-1$ internal edges and contracting the final one, yields a graph $G' = (c_{i,j} \circ l_{i,j}^{1-\rho})(G)$ whose symmetry factor is related to that of the graph $G \in \mathcal{C}$ via $S^{G'} = \frac{1}{\rho!} S^{\mathcal{C}}$. Let $\hat{\theta}^{n-1,k+1-\rho,s} = \sum_{G' \in V_{\text{loopless}}^{n-1,k+1-\rho,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$.

Let $\mathcal{B} \subseteq V_{\text{loopless}}^{n-1,k+1-\rho,s}$ denote the equivalence class containing G' . Applying the $q_i^{(\rho)}$ -map to the graph G' produces a graph isomorphic to the graph G with coefficient $\alpha'_G = \frac{\beta_{G'}}{(\rho-1)!} \in \mathbb{Q}$. Each vertex of the graph G' has at least one labeled external edge. Hence, by induction assumption, $\sum_{G' \in \mathcal{B}} \beta_{G'} = 1/S^{G'} = 1/S^{\mathcal{B}}$. Now, take one graph (distinct from G) in \mathcal{C} in turn, choose one of the internal edges connected to the vertex having r external edges whose free ends are labeled x_{a_1}, \dots, x_{a_r} , and to the vertex having r' external edges whose free ends

are labeled $x_{b_1}, \dots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\sum_{G \in \mathcal{C}} \alpha'_G = \frac{1}{(\rho-1)!} \sum_{G' \in \mathcal{B}} \beta_{G'} = \frac{1}{(\rho-1)! S^{\mathcal{B}}} = \frac{\rho}{S^{\mathcal{C}}}.$$

Therefore, the contribution to $\sum_{G \in \mathcal{C}} \alpha_G$ is $\rho/(m \cdot S^{\mathcal{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m \cdot S^{\mathcal{C}})$ for each edge.

We conclude that every one of the m internal edges of the graph G contributes with a factor of $1/(m \cdot S^{\mathcal{C}})$ to $\sum_{G \in \mathcal{C}} \alpha_G$. Hence, the overall contribution is exactly $1/S^{\mathcal{C}}$. This completes the proof. \square

\square

Appendix D shows the result of computing all mutually non isomorphic connected graphs without external edges as contributions to $\theta^{n,k,0}$ or $\hat{\theta}^{n,k,0}$, for internal edge number $m = k + n - 1 \leq 4$.

4.3.3 Algorithmic considerations

The results of the present section can be seen as an extension of those of Section IV of [6], to loopless connected graphs.

The two algorithms underlying the recursive definitions (1) and (5) given in Sections 3 and 4.3.2, respectively, are amenable for direct implementation using the Hopf algebraic representation of graphs given in [5, 6]. This representation can be used directly and efficiently in implementing concrete calculations of graphs.

An important aspect for the efficiency of concrete calculations is to discard graphs that do not contribute. For instance, assume that one is only interested in calculating loopless graphs so that all vertices have a minimum degree, say, $\nu \geq k + 1$. In particular, in the recursive definition (5), the number of ends of edges assigned to a vertex changes after applying the $q_i^{(\rho)}$ -maps. The only graphs with degree $1 \leq \rho \leq k + 1$ vertices are those produced by the $s_{\mathcal{E}_i}$ -maps when one of the new vertices receives no ends of edges at all. This, thus, acquires degree ρ after being connected to the other vertex with ρ internal edges. Hence, to eliminate the irrelevant graphs with degree $\nu' < \nu$ vertices, replace the $q_i^{(\rho)}$ -maps by $q_i^{(\rho)} \geq \nu := \frac{1}{2(\rho-1)!} l_{i,n+1}^\rho \circ s_{\mathcal{E}_i}^{(\rho)}$ in formula (5), where the $s_{\mathcal{E}_i}^{(\rho)}$ -maps are required to partition the set of ends of edges assigned to the vertex v_i , \mathcal{E}_i , into two sets whose cardinality is equal or greater than $\nu - \rho$.

When considering loop graphs as well, we can no longer globally restrict the image of the maps $q_i^{(1)} = l_{i,n+1} \circ s_{\mathcal{E}_i}$ in formula (1). However, if we are interested in graphs only up to a maximal cyclomatic number, say, k' , we may still restrict the partitions of the set \mathcal{E}_i as part of the definition of the $q_i^{(1)}$ -maps, in certain instances. These are precisely the instances when

a later application of the t_i -maps to a graph cannot occur, i.e., when the graph has already the maximal cyclomatic number k' .

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A

This appendix is the same as that of [6]. It shows $\omega^{n,k,0}$ up to order $n + k \leq 4$ and computed via formula (1). All graphs in the same equivalence class are identified as the same. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

$$n = 1, k = 0 \quad \bullet$$

$$n = 2, k = 0 \quad \frac{1}{2} \quad \bullet \text{---} \bullet$$

$$n = 1, k = 1 \quad \frac{1}{2} \quad \bullet \text{---} \bullet$$

$$n = 3, k = 0 \quad \frac{1}{2} \quad \bullet \text{---} \bullet \text{---} \bullet$$

$$n = 2, k = 1 \quad \frac{1}{2} \quad \bullet \text{---} \bullet + \frac{1}{2^2} \quad \bullet \text{---} \bullet$$

$$n = 1, k = 2 \quad \frac{1}{2^3} \quad \text{---} \circ \text{---}$$

$$n = 4, k = 0 \quad \frac{1}{2} \quad \text{---} \circ \text{---} \circ \text{---} \circ \text{---} \circ + \frac{1}{3!} \quad \begin{array}{c} \circ \\ | \\ \circ \text{---} \circ \\ | \\ \circ \end{array}$$

$$n = 3, k = 1 \quad \frac{1}{3!} \quad \begin{array}{c} \circ \\ / \backslash \\ \circ \text{---} \circ \end{array} + \frac{1}{2^2} \quad \text{---} \circ \text{---} \circ \text{---} \circ + \frac{1}{2} \quad \text{---} \circ \text{---} \circ \text{---} \circ + \frac{1}{2} \quad \text{---} \circ \text{---} \circ \text{---} \circ$$

$$n = 2, k = 2 \quad \frac{1}{2^3} \quad \text{---} \circ \text{---} \circ + \frac{1}{2^3} \quad \text{---} \circ \text{---} \circ \text{---} \circ + \frac{1}{2^2} \quad \text{---} \circ \text{---} \circ \text{---} \circ + \frac{1}{2 \cdot 3!} \quad \text{---} \circ \text{---} \circ \text{---} \circ$$

$$n = 1, k = 3 \quad \frac{1}{2^3 \cdot 3!} \quad \text{---} \circ \text{---} \circ \text{---} \circ$$

B

This appendix shows $\beta^{n,k,0}$ up to order $n + k \leq 5$ and computed via formula (2). All graphs in the same equivalence class are identified as the same. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

$$n = 1, k = 0 \quad \text{---} \circ \text{---}$$

$$n = 1, k = 1 \quad \frac{1}{2} \quad \text{---} \circ \text{---}$$

$$n = 2, k = 1 \quad \frac{1}{2^2} \quad \text{---} \circ \text{---} \circ \text{---}$$

$$n = 1, k = 2 \quad \frac{1}{2^3} \quad \text{---} \text{---} \text{---}$$

$$n = 3, k = 1 \quad \frac{1}{3!} \quad \text{---} \text{---} \text{---}$$

$$n = 2, k = 2 \quad \frac{1}{2^2} \quad \text{---} \text{---} \text{---} + \frac{1}{2 \cdot 3!} \quad \text{---} \text{---} \text{---}$$

$$n = 1, k = 3 \quad \frac{1}{2^3 \cdot 3!} \quad \text{---} \text{---} \text{---}$$

$$n = 4, k = 1 \quad \frac{1}{8} \quad \text{---} \text{---} \text{---}$$

$$n = 3, k = 2 \quad \frac{1}{2^2} \quad \text{---} \text{---} \text{---} + \frac{1}{2^2} \quad \text{---} \text{---} \text{---} + \frac{1}{2^3} \quad \text{---} \text{---} \text{---}$$

$$n = 2, k = 3 \quad \frac{1}{2^4} \quad \text{---} \text{---} \text{---} + \frac{1}{2 \cdot 3!} \quad \text{---} \text{---} \text{---} + \frac{1}{2^4} \quad \text{---} \text{---} \text{---} + \frac{1}{2 \cdot 4!} \quad \text{---} \text{---} \text{---}$$

$$n = 1, k = 4 \quad \frac{1}{2^4 \cdot 4!} \quad \text{---} \text{---} \text{---}$$

C

This appendix shows $\sigma^{n,k,0}$ up to order $n + k \leq 6$ and computed via formula (3). All graphs in the same equivalence class are identified as the same. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

$$n = 1, k = 0 \quad \bullet$$

$$n = 2, k = 0 \quad \frac{1}{2} \quad \bullet - \bullet$$

$$n = 3, k = 0 \quad \frac{1}{2} \quad \bullet - \bullet - \bullet$$

$$n = 4, k = 0 \quad \frac{1}{2} \quad \bullet - \bullet - \bullet - \bullet + \frac{1}{3!} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet \\ | \\ \bullet \end{array}$$

$$n = 3, k = 1 \quad \frac{1}{3!} \quad \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet - \bullet \end{array}$$

$$n = 5, k = 0 \quad \frac{1}{2} \quad \bullet - \bullet - \bullet - \bullet - \bullet + \frac{1}{2} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet \\ | \\ \bullet \end{array} + \frac{1}{4!} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet \\ | \\ \bullet \end{array}$$

$$n = 4, k = 1 \quad \frac{1}{8} \quad \begin{array}{cc} \bullet & \bullet \\ | & | \\ \bullet & \bullet \end{array} + \frac{1}{2} \quad \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet - \bullet - \bullet \\ | \\ \bullet \end{array}$$

$$n = 6, k = 0 \quad \frac{1}{2} \quad \bullet - \bullet - \bullet - \bullet - \bullet - \bullet + \frac{1}{2} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet - \bullet \\ | \\ \bullet \end{array} + \frac{1}{2} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet \\ | \\ \bullet \end{array} \\ + \frac{1}{3!} \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet - \bullet - \bullet \\ | \\ \bullet \end{array} + \frac{1}{2^3} \quad \begin{array}{c} \bullet \quad \bullet \\ | \quad | \\ \bullet - \bullet - \bullet \\ | \quad | \\ \bullet \quad \bullet \end{array} + \frac{1}{5!} \quad \begin{array}{c} \bullet \quad \bullet \\ | \quad | \\ \bullet - \bullet - \bullet \\ | \quad | \\ \bullet \quad \bullet \end{array}$$

$$n = 5, k = 1 \quad \frac{1}{10} \begin{array}{c} \bullet \quad \bullet \\ | \quad | \\ \bullet \quad \bullet \end{array} \bullet + \frac{1}{2} \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array} \bullet + \frac{1}{2} \begin{array}{c} \bullet \\ | \\ \bullet \end{array} \bullet \bullet \bullet + \frac{1}{4} \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array}$$

$$n = 4, k = 2 \quad \frac{1}{4} \begin{array}{c} \bullet \quad \bullet \\ | \quad | \\ \bullet \quad \bullet \end{array}$$

D

This appendix shows $\theta^{n,k,0}$ or $\hat{\theta}^{n,k,0}$ up to order $n + k \leq 5$ and computed via formulas (4) or (5), respectively. All graphs in the same equivalence class are identified as the same. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

$$n = 1, k = 0 \quad \bullet$$

$$n = 2, k = 0 \quad \frac{1}{2} \bullet \bullet$$

$$n = 3, k = 0 \quad \frac{1}{2} \bullet \bullet \bullet$$

$$n = 2, k = 1 \quad \frac{1}{2^2} \bullet \bullet$$

$$n = 4, k = 0 \quad \frac{1}{2} \bullet \bullet \bullet \bullet + \frac{1}{3!} \begin{array}{c} \bullet \\ | \\ \bullet \end{array} \bullet \bullet$$

$$k = 1, n = 3 \quad \frac{1}{3!} \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array} + \frac{1}{2} \bullet \bullet \bullet$$

$$n = 2, k = 2 \quad \frac{1}{2 \cdot 3!} \bullet \bullet$$

$$\begin{aligned}
n = 5, k = 0 & \quad \frac{1}{2} \text{ --- } + \frac{1}{2} \text{ --- } + \frac{1}{4!} \text{ ---} \\
n = 4, k = 1 & \quad \frac{1}{8} \text{ --- } + \frac{1}{2} \text{ --- } + \frac{1}{4} \text{ --- } + \frac{1}{2} \text{ --- } \\
& \quad + \frac{1}{4} \text{ ---} \\
n = 3, k = 2 & \quad \frac{1}{2^2} \text{ --- } + \frac{1}{2^3} \text{ --- } + \frac{1}{3!} \text{ ---} \\
n = 2, k = 3 & \quad \frac{1}{2 \cdot 4!} \text{ ---}
\end{aligned}$$

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